

## AUTHOR INDEX TO VOLUME 142

Abed, K.J. and S. Clough, Methyl tunnelling rotation in the *n*-alkanes 142 (1987) 209

Al Sadoun, M., see M. Madru 142 (1987) 103

Amos, R.D., see K.J. Jalkanen 142 (1987) 153

André, J.-J., see M. Madru 142 (1987) 103

Andzelm, J., N. Russo and D.R. Salahub, Model potential for As and LCGTO MP LSD calculation of geometry, electronic structure and photoelectron spectra for As<sub>2</sub> and As<sub>4</sub> 142 (1987) 169

Arend, H., see J. Seliger 142 (1987) 334

Asscher, M., see G. Haase 142 (1987) 241

Astill, A.G., A.J. McCaffery and B.J. Whitaker, Optical-optical double resonance spectrum of Na<sub>2</sub>: observation of atomic and molecular ultraviolet emission 142 (1987) 1

Avnir, D., see V.R. Kaufman 142 (1987) 551

Balasubramanian, K., M.Z. Liao and S.H. Lin, CAS SCF/CI calculations of potential energy surfaces of He<sub>3</sub><sup>+</sup> and He<sub>2</sub><sup>+</sup> 142 (1987) 349

Barbier, C., Ab initio calculation of the electric polarizability of infinite chains by the Genkin-Mednis approach. Preliminary investigation on model chains of hydrogen molecules 142 (1987) 53

Barnes, A.C., J.E. Enderby, J. Breen and J.C. Leyte, The water structure around the chloride ion in aqueous polyethylene oxide solutions 142 (1987) 405

Bartels, D.M., D.W. Werst and A.D. Trifunac, H atom diffusion and CIDEP in room temperature fused silica 142 (1987) 191

Bartlett, R.J., see S. Pal 142 (1987) 575

Barzen, K., P. Wollenweber and H. Schmoranzer, Empirical determination of the potential curves of the ground state and the first two excited states of Kr<sub>2</sub> 142 (1987) 79

Bauder, A., see M. Rodler 142 (1987) 10

Bauschlicher Jr., C.W., How important is correlation in the description of the Ni-H<sub>2</sub>O interaction 142 (1987) 71

Bausk, N.V., see A.V. Kondratenko 142 (1987) 509

Becker, A.C. and U. Schurath, Matrix-isolated NF: radiative rates of b<sup>1</sup>Σ<sup>+</sup>→a<sup>1</sup>Δ, b<sup>1</sup>Σ<sup>+</sup>→X<sup>3</sup>Σ<sup>-</sup>, and a<sup>1</sup>Δ→X<sup>3</sup>Σ<sup>-</sup>, in solid argon 142 (1987) 313

Bell, T.N., see I. Safarik 142 (1987) 115

Bisht, P.B., G.C. Joshi, H.B. Tripathi and D.D. Pant, Time-resolved spectroscopy of 2-naphthol-triethylamine charge-transfer complexes in polar and non-polar solvents 142 (1987) 291

Bist, H.D., see P.S.R. Prasad 142 (1987) 341

Black, G., T. Nishiya, H. Shinohara, N. Nishi and I. Hanazaki, REMPI studies in the Lewis-Rayleigh afterglow of nitrogen 142 (1987) 409

Blinc, R., see J. Seliger 142 (1987) 334

Bondybey, V.E., see M. Rasanen 142 (1987) 308

Brauman, J.I., see H. Tanaka 142 (1987) 371

Bréchignac, Ph., N. Halberstadt, B.J. Whitaker and B. Coutant, Infrared predissociation of (NO)<sub>2</sub>: rotational distribution of the fragments 142 (1987) 125

Breen, J., see A.C. Barnes	142 (1987) 405
Brocklehurst, B. and D.B. Cook, The muonium bond	142 (1987) 329
Brooks III, C.L., see D.J. Tobias	142 (1987) 472
Brown, C.E., J.J. Orlando, J. Reid and D.R. Smith, Diode laser detection of transient $\text{CF}_3$ radicals formed by $\text{CO}_2$ laser multiphoton induced dissociation of halocarbons	142 (1987) 213
Buma, W.J., R.G. Evelo, E.J.J. Groenen, A.J. Hoff, H.M. Nan and J. Schmidt, The reaction center triplet state of the photosynthetic bacterium <i>Rhodobacter sphaeroides</i> R26: electron spin echo spectroscopy of a single crystal	142 (1987) 231
Burns, W.G. and A. Mozumder, Theoretical analysis of free-ion yield in liquid argon under low-LET irradiation	142 (1987) 381
Cardini, G., G.F. Signorini, P.R. Salvi and R. Righini, Molecular dynamics and head-tail disorder in the Raman spectrum of crystalline $\text{N}_2\text{O}$	142 (1987) 570
Castiglioni, C., see M. Gussoni	142 (1987) 515
Chakravorty, S.J. and S.R. Gadre, Coulomb energy, total X-ray scattering intensities and average electron densities	142 (1987) 205
Chang, R.S.F., see J.D. Stanfill	142 (1987) 275
Chowdhury, P.K., J. Pola, K.V.S. Rama Rao and J.P. Mittal, TEA $\text{CO}_2$ laser driven oxidation of tetrafluoroethene and decafluorocyclopentane with molecular oxygen. Evidence for the dioxetane mechanism	142 (1987) 252
Clarisse, C., see M. Madru	142 (1987) 103
Clifford, P., see A. Mozumder	142 (1987) 385
Clough, S., see K.J. Abed	142 (1987) 209
Connell, L.L., see P.M. Felker	142 (1987) 439
Cook, D.B., see B. Brocklehurst	142 (1987) 329
Corcoran, T.C., see P.M. Felker	142 (1987) 439
Coutant, B., see Ph. Bréchignac	142 (1987) 125
Crosby, G.A., see C.A. Helms	142 (1987) 99
Dalvi, A.G.I., see M.D. Sastry	142 (1987) 280
Danchura, W., see B.A. Pettitt	142 (1987) 455
Davis, M.J., see C.C. Martens	142 (1987) 519
De Boer, S., see K.J. Vink	142 (1987) 433
De Levie, R., see R. Sridharan	142 (1987) 43
Deng, C., see B. Wang	142 (1987) 92
Derouane, E.G., The energetics of sorption by molecular sieves: surface curvature effects	142 (1987) 200
Desmarest, P., R. Tufeu, Y. Garrabos and B. le Neindre, Decay rate of critical fluctuations in steam along the critical isochore	142 (1987) 336
Djeu, N., see J.D. Stanfill	142 (1987) 275
Drewello, T., see W. Koch	142 (1987) 147
Dubs, R.L. and V. McKoy, Studies of $\text{NiN}_2$ as a model for photoemission from $\text{N}_2$ adsorbed on nickel	142 (1987) 237
Dupuis, M., see H.O. Villar	142 (1987) 59
Durant, J.L. and F. Kaufman, Calculation and use of total collision rates in thermal systems	142 (1987) 246
Dyke, T.R., see M.A. Walsh	142 (1987) 265
Dzugan, T.P., see M. Rasanen	142 (1987) 308

Eaton, G.R., see S.S. Eaton	142 (1987) 567
Eaton, S.S., M.M. Maltempo, E.D.A. Stemp and G.R. Eaton, Three-dimensional EPR imaging with one spectral and two spatial dimensions	142 (1987) 567
Eicke, H.-F. and J. Naudts, Non-linear field effects due to activation-energy-controlled charge transport in microemulsions	142 (1987) 106
Enderby, J.E., see A.C. Barnes	142 (1987) 405
England, T.H., see M.A. Walsh	142 (1987) 265
Evelo, R.G., see W.J. Buma	142 (1987) 231
Ezra, G.S., see B.G. Sumpter	142 (1987) 142
Ezra, G.S., see C.C. Martens	142 (1987) 519
Fantucci, P., see G. Pacchioni	142 (1987) 85
Fayer, M.D., see H. Tanaka	142 (1987) 371
Felker, P.M., B.F. Henson, T.C. Corcoran, L.L. Connell and G.V. Hartland, Fourier transform stimulated emission pumping spectroscopy	142 (1987) 439
Ferrer, I.J. and P. Salvador, Mechanisms of photoluminescence at CdS polycrystalline electrodes in contact with aqueous electrolytes	142 (1987) 399
Fidy, J., H. Koloczek, K.-G. Paul and J.M. Vanderkooi, The <i>pH</i> dependence of phototautomerism in horse radish peroxidase monitored by fluorescence site-selection spectroscopy	142 (1987) 562
Flores, J.R. and J. Largo-Cabrero, A comparative ab initio study of the $\text{H}_2\text{SiN}^+$ and $\text{H}_2\text{CN}^+$ cations	142 (1987) 159
Freedman, A., K.E. McCurdy, J. Wormhoudt and P.P. Gaspar, Temperature dependence of gas phase reactions of $\text{SiF}_2$ with $\text{F}_2$ and $\text{Cl}_2$	142 (1987) 255
Gadre, S.R., see S.J. Chakravorty	142 (1987) 205
Garrabos, Y., see P. Desmarest	142 (1987) 336
Gaspar, P.P., see A. Freedman	142 (1987) 255
George, T.F., see I. Last	142 (1987) 19
Gien, T.T., Core-corrected modified Glauber approximation for $e^\pm$ -alkali-metal-atom collisions, Chem. Phys. Letters 139 (1987) 23. Erratum	142 (1987) 575
Gilchrist, J. le G., Dielectric relaxations in partly deuterated ammonium dichromate	142 (1987) 121
Golde, M.F., see R.F. Sperlein	142 (1987) 359
Golovko, M.F. and I.A. Protsykevich, Pair correlation functions for the asymmetric ion-dipole model in the mean spherical approximation	142 (1987) 463
Gordon, M.S. and T.N. Truong, Potential primary pyrolysis processes of methylsilane	142 (1987) 110
Green, N.J.B., see A. Mozumder	142 (1987) 385
Griffiths, W.J. and F.M. Harris, Ionization energies of $\text{CH}_3\text{O}^-$ and $\text{CH}_3\text{S}^-$ radicals measured by charge-inversion energy-loss spectrometry	142 (1987) 7
Groenen, E.J.J., see W.J. Buma	142 (1987) 231
Guillaud, G., see M. Madru	142 (1987) 103
Guillory, W.A., see B. Hoesterey	142 (1987) 261
Günter, P., see J. Seliger	142 (1987) 334
Gussoni, M., M.N. Ramos, C. Castiglioni and G. Zerbi, Ab initio counterpart of infrared atomic charges	142 (1987) 515
Haase, G. and M. Asscher, Interaction of $\text{N}_2$ with $\text{Re}(11\bar{2}0)$ in the presence of $\text{H}_2$	142 (1987) 241

Hackett, P.A., see Y. Ishikawa	142 (1987) 271
Halberstadt, N., see Ph. Bréchignac	142 (1987) 125
Halpern, B. and M. Kori, Statistical energy partitioning in surface reactions: the Pt-catalyzed oxidations of C and CO, <i>Chem. Phys. Letters</i> 138 (1987) 261. Erratum	142 (1987) 302
Hammer, R.E. and K.M. Sando, Valence effective Hamiltonian method for molecular fragments	142 (1987) 48
Hanazaki, I., see G. Black	142 (1987) 409
Handy, N.C., see K.J. Jalkanen	142 (1987) 153
Harris, F.M., see W.J. Griffiths	142 (1987) 7
Hartland, G.V., see P.M. Felker	142 (1987) 439
Hase, W.L., see D. Lu	142 (1987) 187
Hayamizu, K., see T. Uemura	142 (1987) 423
Heather, R., X.-P. Jiang and H. Metiu, The use of Raman spectroscopy to study photo-dissociation dynamics for systems where curve crossing is important	142 (1987) 303
Helms, C.A., T.A. Reynolds and G.A. Crosby, External magnetic field effects on the excited states of iridium(I) and rhodium(I) complexes	142 (1987) 99
Henson, B.F., see P.M. Felker	142 (1987) 439
Herzfeld, J., Closed-form ground state expression for the chemical shift tensor	142 (1987) 469
Hiramatsu, M., R. Nakagaki, Y. Tanimoto, K. Mutai, H. Tukada and S. Nagakura, Intramolecular photo-oxidation of triphenylphosphine and 10-alkylphenothiazine by nitroaromatic moieties: magnetic field effects and long-range oxygen transfer	142 (1987) 413
Hitchman, M.A., see R.G. McDonald	142 (1987) 529
Hoesterey, B., M.B. Mitchell and W.A. Guillory, The triplet state IR spectrum of matrix-isolated anthracene	142 (1987) 261
Hoff, A.J., see W.J. Buma	142 (1987) 231
Hoff, A.J., see K.J. Vink	142 (1987) 433
Hoffmann, M.R. and J. Simons, Analytical energy gradients for a unitary coupled-cluster theory	142 (1987) 451
Hofmann, R.E.S. and M. Holz, Nuclear magnetic relaxation of ionic nuclei moving in an external electric field	142 (1987) 492
Holz, M., see R.E.S. Hofmann	142 (1987) 492
Hopkins, J.B. and P.M. Rentzepis, Picosecond measurements of vibrational energy decay in matrix-isolated polyatomic molecules	142 (1987) 503
Howard, B.J., see M.A. Walsh	142 (1987) 265
Howard, R.E., T.L. Plank, S.R. Trussell and B. Saadevandi, Quasiclassical trajectory calculation of argon-argon recombination rates	142 (1987) 33
Huang, M.B., Some low-lying ionized states of $\text{BeF}_2$ studied by means of the EOM/propagator method	142 (1987) 165
I'Haya, Y.J., see H. Ito	142 (1987) 25
Ishikawa, Y., R.A. Weersink, P.A. Hackett and D.M. Rayner, The dihydrogen complex $\text{W}(\text{CO})_5(\text{H}_2)$ in the gas phase	142 (1987) 271
Ito, H. and Y.J. I'Haya, A polarizability theory for Z-DNA: UV absorption and CD band-shape calculations for the B-to-Z transition of $\text{poly}(\text{dG-dC}) \cdot \text{Poly}(\text{dG-dC})$	142 (1987) 25
Ito, M., see F. Kitamura	142 (1987) 318
Itoh, K., see Y. Teki	142 (1987) 181

Jacobsen, C.S., see H. Toftlund	142 (1987) 286
Jacques, P., Quenching of triplet benzophenone by electron donors: does the linear inverse relation $\ln k_q$ versus IP really work?	142 (1987) 96
Jalkanen, K.J., P.J. Stephens, R.D. Amos and N.C. Handy, Basis set dependence of ab initio predictions of vibrational rotational strengths: NHDT	142 (1987) 153
Jans-Bürli, S., see M. Rodler	142 (1987) 10
Jayanth Kumar, M.L., see M.D. Sastry	142 (1987) 280
Jiang, X.-P., see R. Heather	142 (1987) 303
Jodhan, A., see I. Safarik	142 (1987) 115
Jordan, K.D., see R.F. Sperlein	142 (1987) 359
Joshi, G.C., see P.B. Bisht	142 (1987) 291
 Kaufman, F., see J.L. Durant	142 (1987) 246
Kaufman, V.R., S.C. Müller, K.H. Müller and D. Avnir, Early stages of the silicon alkoxide sol/gel polymerization as detected by dynamic light scattering	142 (1987) 551
Khundkar, L.R. and A.H. Zewail, Picosecond MPI mass spectrometry of $\text{CH}_3\text{I}$ in the process of dissociation	142 (1987) 426
Kitamura, F., M. Takeda, M. Takahashi and M. Ito, CO adsorption on Pt(111) and Pt(100) single crystal surfaces in aqueous solutions studied by infrared reflection-absorption spectroscopy	142 (1987) 318
Kitano, M., see Y. Teki	142 (1987) 181
Kitao, O., see H. Nakatsuji	142 (1987) 446
Kjellander, R. and S. Marčelja, Electrolyte solutions between uncharged walls	142 (1987) 485
Klein, M.L., see J.S. Tse	142 (1987) 175
Koch, W., B. Liu, T. Weiske, C.B. Lebrilla, T. Drewello and H. Schwarz, The $\text{CH}^{2+}$ dication: metastable or not? A combined theoretical and experimental investigation	142 (1987) 147
Kohse-Höinghaus, K., see U. Meier	142 (1987) 498
Kokai, F., see H. Tanaka	142 (1987) 371
Koloczek, H., see J. Fidy	142 (1987) 562
Komori, M., see H. Nakatsuji	142 (1987) 446
Kondratenko, A.V., V.I. Nemanova, N.V. Bausk, L.N. Mazalov, S.F. Ruzankin and G.M. Zhydomirov, An SCF $X\alpha$ SW calculation of Pt X-ray absorption spectra in chloride complexes: pre-edge structure, XANES and EXAFS	142 (1987) 509
Koos, D.A., see V.L. Shannon	142 (1987) 323
Kori, M., see B. Halpern	142 (1987) 302
Koszykowski, M.L., C.M. Rohlfing and D.W. Noid, The use of ab initio electronic structure energies in the semi-classical calculation of vibrational spectra	142 (1987) 67
Koutecký, J., see G. Pacchioni	142 (1987) 85
Kumar, V., A.K. Rai, S.N. Thakur and D.K. Rai, Population monitoring in the B-X system of HgBr by laser optogalvanic spectroscopy	142 (1987) 217
 Largo-Cabrero, J., see J.R. Flores	142 (1987) 159
Last, I. and T.F. George, Light absorption by an atom moving inside a spherical box	142 (1987) 19
Lebrilla, C.B., see W. Koch	142 (1987) 147
Le Contellec, M., see M. Madru	142 (1987) 103
Le Neindre, B., see P. Desmarest	142 (1987) 336
Leyte, J.C., see A.C. Barnes	142 (1987) 405

Liao, M.Z., see K. Balasubramanian	142 (1987) 349
Lim, E.C., see P.-N. Wang	142 (1987) 389
Lin, S.H., see K. Balasubramanian	142 (1987) 349
Liu, B., see W. Koch	142 (1987) 147
Liu, J.Y., see M. Rasanen	142 (1987) 308
Lu, D. and W.L. Hase, Quasiclassical trajectory study of the $n=3$ overtone state of benzene	142 (1987) 187
Madru, M., G. Guillaud, M. Al Sadoun, M. Maitrot, C. Clarisse, M. le Contellec, J.-J. André and J. Simon, The first field effect transistor based on an intrinsic molecular semiconductor	142 (1987) 103
Maitrot, M., see M. Madru	142 (1987) 103
Maltempo, M.M., see S.S. Eaton	142 (1987) 567
Marcelja, S., see R. Kjellander	142 (1987) 485
Martens, C.C., M.J. Davis and G.S. Ezra, Local frequency analysis of chaotic motion in multidimensional systems: energy transport and bottlenecks in planar OCS	142 (1987) 519
Maynard, K.J. and M. Moskovits, Carbon monoxide adsorption on alkali metal predosed silver surfaces	142 (1987) 298
Mazalov, L.N., see A.V. Kondratenko	142 (1987) 509
McCaffery, A.J., see A.G. Astill	142 (1987) 1
McCurdy, K.E., see A. Freedman	142 (1987) 255
McDonald, R.G., M.J. Riley and M.A. Hitchman, Derivation of a system of "hot" bands from the electronic spectrum of planar $\text{CuCl}_2^-$ : Evidence for a pseudo-tetrahedral distortion in the $^2\text{A}_{1g}$ excited electronic state	142 (1987) 529
McDouall, J.J.W. and M.A. Robb, The transformation of CAS SCF wavefunctions to valence bond space	142 (1987) 131
McKoy, V., see R.L. Dubs	142 (1987) 237
Meier, U. and K. Kohse-Höinghaus, REMPI detection of $\text{CH}_3$ in low-pressure flames	142 (1987) 498
Menzel, R. and P. Witte, Photophysical hole burning in the excited-state absorption bands of dissolved organic molecules at room temperature	142 (1987) 366
Merchán, M., see J. Miralles-Sabater	142 (1987) 136
Messer, B. and H. Tributsch, Silicon-hydrogen interaction seen by microwave-photo-electrochemical techniques	142 (1987) 546
Metiu, H., see R. Heather	142 (1987) 303
Miralles-Sabater, J., M. Merchán and I. Nebot-Gil, A CI study of the $\text{Al}/\text{C}_2\text{H}_2$ and $\text{Al}/\text{C}_2\text{H}_4$ $\pi$ complexes	142 (1987) 136
Mitchell, M.B., see B. Hoesterey	142 (1987) 261
Mittal, J.P., see P.K. Chowdhury	142 (1987) 252
Monkhouse, P., see R. Schwarzwald	142 (1987) 15
Moskovits, M., see K.J. Maynard	142 (1987) 298
Mozumder, A., see W.G. Burns	142 (1987) 381
Mozumder, A., S.M. Pimblott, P. Clifford and N.J.B. Green, Electron-ion geminate escape probability in anisotropic media	142 (1987) 385
Mukherjee, D., see S. Pal	142 (1987) 575
Müller, K.H., see V.R. Kaufman	142 (1987) 551
Müller, S.C., see V.R. Kaufman	142 (1987) 551
Mutai, K., see M. Hiramatsu	142 (1987) 413

Nagakura, S., see M. Hiramatsu	142 (1987) 413
Nakagaki, R., see M. Hiramatsu	142 (1987) 413
Nakamura, H., see A. Ohsaki	142 (1987) 37
Nakatsuji, H., M. Komori and O. Kitao, Cluster expansion of the wavefunction: ionizations and some low-energy excitations of naphthalene	142 (1987) 446
Nan, H.M., see W.J. Buma	142 (1987) 231
Natarajan, V., see M.D. Sastry	142 (1987) 280
Naudts, J., see H.-F. Eicke	142 (1987) 106
Nebot-Gil, I., see J. Miralles-Sabater	142 (1987) 136
Nemanova, V.I., see A.V. Kondratenko	142 (1987) 509
Niccolai, N., see C. Rossi	142 (1987) 418
Nishi, N., see G. Black	142 (1987) 409
Nishiya, T., see G. Black	142 (1987) 409
Noid, D.W., see M.L. Koszykowski	142 (1987) 67
Ohsaki, A. and H. Nakamura, Approximate quantum mechanical treatment of light-atom transfer reactions	142 (1987) 37
Okuno, Y., see T. Uemura	142 (1987) 423
Oldani, M., see M. Rodler	142 (1987) 10
Orlando, J.J., see C.E. Brown	142 (1987) 213
Pacchioni, G., P. Fantucci and J. Koutecký, Potential energy surfaces of low-lying states of the aluminum trimer	142 (1987) 85
Pal, S., M. Rittby, R.J. Bartlett, D. Sinha and D. Mukherjee, Multireference coupled-cluster methods using an incomplete model space: application to ionization potentials and excitation energies of formaldehyde, Chem. Phys. Letters 137 (1987) 273. Erratum	142 (1987) 575
Pant, D.D., see P.B. Bisht	142 (1987) 291
Paul, K.-G., see J. Fidy	142 (1987) 562
Peters, N.J.S., Ab initio study of the isoelectronic series $N^-_3$ , $N_2O$ and $N_2F^+$ : predicting the bond lengths in $N_2F^+$	142 (1987) 76
Pettitt, B.A. and W. Danchura, Rovibrational momentum densities of diatomic molecules in the rigid rotor-harmonic oscillator approximation	142 (1987) 455
Pimblott, S.M., see A. Mozumder	142 (1987) 385
Plank, T.L., see R.E. Howard	142 (1987) 33
Plijter, J.J., see K.J. Vink	142 (1987) 433
Pola, J., see P.K. Chowdhury	142 (1987) 252
Prasad, P.S.R., S. Sathaiah and H.D. Bist, Raman spectroscopic study of $(CH_3NH_3)_2HgCl_4$ in the high-temperature range	142 (1987) 341
Protsykevich, I.A., see M.F. Golovko	142 (1987) 463
Rai, A.K., see V. Kumar	142 (1987) 217
Rai, D.K., see V. Kumar	142 (1987) 217
Rama Rao, K.V.S., see P.K. Chowdhury	142 (1987) 252
Ramos, M.N., see M. Gussoni	142 (1987) 515
Rangarajan, S.K., see R. Sridharan	142 (1987) 43
Rasanen, M., J.Y. Liu, T.P. Dzugan and V.E. Bondybey, Matrix studies of the products of laser vaporization of graphite	142 (1987) 308

Rayner, D.M., see Y. Ishikawa	142 (1987) 271
Reid, J., see C.E. Brown	142 (1987) 213
Rentzepis, P.M., see J.B. Hopkins	142 (1987) 503
Reynolds, T.A., see C.A. Helms	142 (1987) 99
Richmond, G.L., see V.L. Shannon	142 (1987) 323
Richter, W., see D. Schiel	142 (1987) 345
Righini, R., see G. Cardini	142 (1987) 570
Riley, M.J., see R.G. McDonald	142 (1987) 529
Rittby, M., see S. Pal	142 (1987) 575
Robb, M.A., see J.J.W. McDouall	142 (1987) 131
Robinson, J.M., see V.L. Shannon	142 (1987) 323
Rodler, M., S. Jans-Bürli, M. Oldani and A. Bauder, Nuclear quadrupole couplings in HNCS and DNCS	142 (1987) 10
Rohlfing, C.M., see M.L. Koszykowski	142 (1987) 67
Rose, J.L., see C. Samet	142 (1987) 557
Rossi, C. and N. Niccolai, The measurement of direct $^1\text{H}$ - $^{13}\text{C}$ dipolar relaxation terms from proton spin-lattice relaxation experiments	142 (1987) 418
Russo, N., see J. Andzelm	142 (1987) 169
Ruzankin, S.F., see A.V. Kondratenko	142 (1987) 509
Saaddevandi, B., see R.E. Howard	142 (1987) 33
Safarik, I., A. Jodhan, O.P. Strausz and T.N. Bell, $\text{Hg}({}^3\text{P}_1)$ photosensitization of trimethylsilane in the presence of alcohol	142 (1987) 115
Salahub, D.R., see J. Andzelm	142 (1987) 169
Salvador, P., see I.J. Ferrer	142 (1987) 399
Salvi, P.R., see G. Cardini	142 (1987) 570
Samet, C., J.L. Rose, B.E. Williamson and P.N. Schatz, Magnetic circular dichroism of the potassium atom "blue triplet" in a xenon matrix	142 (1987) 557
Sando, K.M., see R.E. Hammer	142 (1987) 48
Sastry, M.D., V. Natarajan, A.G.I. Dalvi and M.L. Jayanth Kumar, Electron paramagnetic resonance of $^{241}\text{Am}$ with a $5\text{f}^67\text{s}^1$ configuration in a $\text{BaCO}_3$ lattice	142 (1987) 280
Sathaiah, S., see P.S.R. Prasad	142 (1987) 341
Schaefer III, H.F., see G.E. Scuseria	142 (1987) 354
Schatz, P.N., see C. Samet	142 (1987) 557
Schiel, D. and W. Richter, The OH-stretching vibrational Raman profile and isomer assignment of 2-propanol	142 (1987) 345
Schipper, P.E., A passive-pair simplified group function analysis of aromaticity: application to electronic superconductivity	142 (1987) 393
Schmidt, J., see W.J. Buma	142 (1987) 231
Schmoranzer, H., see K. Barzen	142 (1987) 79
Schurath, U., see A.C. Becker	142 (1987) 313
Schwarz, H., see W. Koch	142 (1987) 147
Schwarzwald, R., P. Monkhouse and J. Wolfrum, Picosecond fluorescence lifetime measurement of the OH radical in an atmospheric pressure flame	142 (1987) 15
Scuseria, G.E. and H.F. Schaefer III, The optimization of molecular orbitals for coupled cluster wavefunctions	142 (1987) 354
Seliger, J., V. Žagar, R. Blinc, H. Arend and P. Günter, $^{14}\text{N}$ quadrupole coupling in COANP	142 (1987) 334
Shannon, V.L., D.A. Koos, J.M. Robinson and G.L. Richmond, Optical second-harmonic generation as an in situ probe of electrode surface dynamics. Ag(111)	142 (1987) 323

Sheng, R., Identification of the Kekulé structures of a hexagonal system	142 (1987) 196
Shinohara, H., see G. Black	142 (1987) 409
Signorini, G.F., see G. Cardini	142 (1987) 570
Silverman, J.N., Physical origins of high-order Born-Oppenheimer electronic polarizabilities: application to a 30th-order perturbation study of $H_2^+$	142 (1987) 477
Simon, J., see M. Madru	142 (1987) 103
Simons, J., see M.R. Hoffmann	142 (1987) 451
Sinha, D., see S. Pal	142 (1987) 575
Slanina, Z., Comparing theoretical and observed data in the $C_6(g)$ system	142 (1987) 512
Smith, D.R., see C.E. Brown	142 (1987) 213
Sperlein, R.F., M.F. Golde and K.D. Jordan, Ab initio study of electronic energy transfer in the quenching of $CO^*(a^3\Pi)$ by $H_2$	142 (1987) 359
Sridharan, R., R. de Levie and S.K. Rangarajan, Two-dimensional phase transitions at electrochemical interfaces	142 (1987) 43
Stanfill, J.D., R.S.F. Chang and N. Djeu, Electronic energy transfer from $Mg(^3P)$ to Sm	142 (1987) 275
Stemp, E.D.A., see S.S. Eaton	142 (1987) 567
Stephens, P.J., see K.J. Jalkanen	142 (1987) 153
Strausz, O.P., see I. Safarik	142 (1987) 115
Sumpter, B.G. and G.S. Ezra, Semiclassical rotation-vibration energies for a triatomic molecule: $H_2O$	142 (1987) 142
Tait, C.D., T.M. Vess and D.W. Wertz, A non-aqueous SERS study of the 2,2'-bipyridine free ligand and the tris(bpy) Ru(II) complex reduction products	142 (1987) 225
Takahashi, M., see F. Kitamura	142 (1987) 318
Takeda, M., see F. Kitamura	142 (1987) 318
Takui, T., see Y. Teki	142 (1987) 181
Tanaka, H., F. Kokai, J.I. Brauman and M.D. Fayer, Effect of hydrogen bond strength on resorufin non-photochemical hole burning in ethanol-2,2,2-trifluoroethanol glasses	142 (1987) 371
Tanimoto, Y., see M. Hiramatsu	142 (1987) 413
Teki, Y., T. Takui, M. Kitano and K. Itoh, Spin alignment in organic high-spin molecules. A Heisenberg Hamiltonian approach	142 (1987) 181
Thakur, S.N., see V. Kumar	142 (1987) 217
Tobias, D.J. and C.L. Brooks III, Calculation of free energy surfaces using the methods of thermodynamic perturbation theory	142 (1987) 472
Toftlund, H., P. Waage Jensen and C.S. Jacobsen, Evidence for $d^7$ defects in linear-chain mixed-valence palladium(II),(IV) complexes of trans-1,2-cyclohexanediamine	142 (1987) 286
Tomohiro, T., see T. Uemura	142 (1987) 423
Tributsch, H., see B. Messer	142 (1987) 546
Trifunac, A.D., see D.M. Bartels	142 (1987) 191
Tripathi, H.B., see P.B. Bisht	142 (1987) 291
Truong, T.N., see M.S. Gordon	142 (1987) 110
Trussell, S.R., see R.E. Howard	142 (1987) 33
Tse, J.S. and M.L. Klein, Molecular dynamics calculation of the infrared and Raman spectra of ice IX in the translational mode region	142 (1987) 175
Tufeu, R., see P. Desmarest	142 (1987) 336
Tukada, H., see M. Hiramatsu	142 (1987) 413

Uemura, T., T. Tomohiro, K. Hayamizu and Y. Okuno, Electron spin resonance of Pt(III) in anticancer platinum pyrimidine green	142 (1987) 423
Van den Berg, R., H. van der Laan and S. Völker, Zeeman effects in amorphous solids: a hole-burning study of free-base porphin in polyethylene	142 (1987) 535
Vanderkooi, J.M., see J. Fidy	142 (1987) 562
Van der Laan, H., see R. van den Berg	142 (1987) 535
Vess, T.M., see C.D. Tait	142 (1987) 225
Villar, H.O. and M. Dupuis, Bond orders and valencies from ab initio wavefunctions: application to prototypical molecules and to the characterization of solitons in polyenes	142 (1987) 59
Vink, K.J., S. de Boer, J.J. Plijter, A.J. Hoff and D.A. Wiersma, Optical dynamics of the reaction center of photosystem II. A hole-burning and photon-echo study	142 (1987) 433
Völker, S., see R. van den Berg	142 (1987) 535
Waage Jensen, P., see H. Toftlund	142 (1987) 286
Walsh, M.A., T.H. England, T.R. Dyke and B.J. Howard, Pulsed molecular beam infrared absorption spectroscopy of CO <sub>2</sub> dimer	142 (1987) 265
Wang, B. and C. Deng, Mechanism of the isomerization of azirinylidene to ketenimine	142 (1987) 92
Wang, P.-N. and E.C. Lim, Time-resolved fluorescence polarization as a probe of the rotational dynamics of electronically excited molecules: fluorescence from single rotational ( <i>J</i> ) level of jet-cooled 0 <sub>0</sub> <sup>0</sup> 1B <sub>1</sub> pyrimidine	142 (1987) 389
Weersink, R.A., see Y. Ishikawa	142 (1987) 271
Weiske, T., see W. Koch	142 (1987) 147
Werst, D.W., see D.M. Bartels	142 (1987) 191
Wertz, D.W., see C.D. Tait	142 (1987) 225
Whitaker, B.J., see A.G. Astill	142 (1987) 1
Whitaker, B.J., see Ph. Bréchignac	142 (1987) 125
White, J.M., see X.-L. Zhou	142 (1987) 376
Wiersma, D.A., see K.J. Vink	142 (1987) 433
Williamson, B.E., see C. Samet	142 (1987) 557
Witte, P., see R. Menzel	142 (1987) 366
Wolfrum, J., see R. Schwarzwald	142 (1987) 15
Wollenweber, P., see K. Barzen	142 (1987) 79
Wormhoudt, J., see A. Freedman	142 (1987) 255
Žagar, V., see J. Seliger	142 (1987) 334
Zerbi, G., see M. Gussoni	142 (1987) 515
Zewail, A.H., see L.R. Khundkar	142 (1987) 426
Zhou, X.-L. and J.M. White, Decomposition kinetics of CH <sub>3</sub> (CD <sub>3</sub> ) on Ni(100)	142 (1987) 376
Zhydomirov, G.M., see A.V. Kondratenko	142 (1987) 509

